3-Chloro-2-fluorobenzoic acid, tetradecyl ester

Inchi: InChI=1S/C21H32ClFO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-17-25-21(24)18-15-14-16-19(22
InchiKey: QRWLCYZEZXKQKY-UHFFFAOYSA-N
Formula: C21H32ClFO2
SMILES: CCCCCCCCCCCCCCOC(=O)c1cccc(Cl)c1F
Mol. weight [g/mol]: 370.93

Physical Properties

Property code	Value	Unit	Source
gf	-221.57	kJ/mol	Joback Method
hf	-719.83	kJ/mol	Joback Method
hfus	53.47	kJ/mol	Joback Method
hvap	78.66	kJ/mol	Joback Method
log10ws	-8.17		Crippen Method
logp	7.337		Crippen Method
mcvol	304.440	ml/mol	McGowan Method
pc	1134.43	kPa	Joback Method
rinpol	2624.00		NIST Webbook
rinpol	2624.00		NIST Webbook
tb	829.51	K	Joback Method
tc	1023.33	K	Joback Method
tf	480.56	K	Joback Method
vc	1.194	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	923.28	J/mol×K	829.51	Joback Method
cpg	940.14	J/mol×K	861.81	Joback Method
cpg	955.97	J/mol×K	894.12	Joback Method
cpg	970.79	J/mol×K	926.42	Joback Method
cpg	984.64	J/mol×K	958.72	Joback Method
cpg	997.57	J/mol×K	991.03	Joback Method
cpg	1009.59	J/mol×K	1023.33	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338891&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume